Structure

In This Issue

CellPress

Safeguarding Repositories of Structural Data

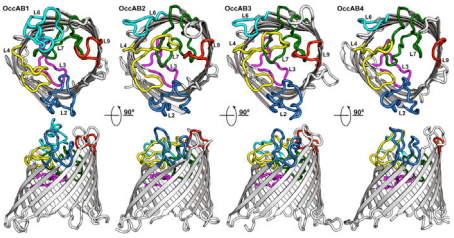
PAGE 216

Structural biology research generates large amounts of data, some deposited in public databases and repositories. The inconsistencies and flaws in depositions may bias data mining and may also affect reproducibility of the results. Minor et al. now propose some solutions and encourage further discussion leading to practical action.

A Broad Look at the Outer Membrane Permeability

PAGE 221

Antibiotic resistance in the Gram-negative bacterium *Acinetobacter baumannii* is caused in part by a low-permeability outer membrane (OM). Zahn et al. combine structural and functional analysis of the OM channels OccAB1-OccAB4 to reveal differences in pore sizes and substrate translocation properties, and they single out OccAB1 as the most promising candidate for targeting by future antibiotics.



Fine-Tuning N-End Rule

PAGE 232

The ClpS adaptor is responsible for delivering N-end rule substrates to ClpAP for degradation in bacteria. Stein et al. present biochemical and structural evidence that *A. tumefaciens* employ an additional more selective ClpS protein, ClpS2, allowing fine-tuning of N-end rule recognition and unfolding/degradation.

Looking Down the Core of β-Barrel Assembly Machine

PAGE 243

Insertion and folding of β-barrel proteins into the bacterial outer membrane is carried out by the β-barrel assembly machine (BAM) complex. Bergal et al. elucidate the crystal structure of a BamA-BamD fusion and present a model of the BamABCD core complex.

Arpin Wags the Tail

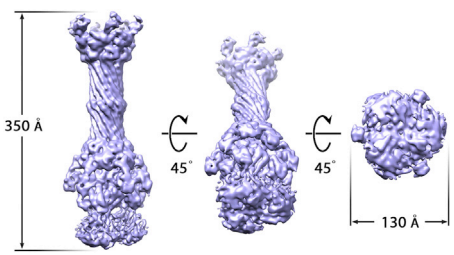
PAGE 252

Arpin is a newly discovered regulator of actin polymerization, which steers cell migration by exerting a negative control on the Arp2/3 complex. Fetics et al. show that C-terminal acidic tail of Arpin is its primary epitope and discuss how Arpin might use it to compete with VCA domains for binding to Arp2/3.

Voltage Sensor in Control of the Gate

PAGE 261

Voltage-gated calcium channels (CaV) translate membrane depolarization into calcium influx that regulates muscle contraction, hormone secretion, or synaptic transmission. Using computational structural modeling, site-directed mutagenesis, and electrophysiology, Tuluc et al. identify the mechanism responsible for different voltage sensitivity of two CaV1.1 calcium channel splice variants.



AcrA and TolC Communicate via Intermeshing Cogwheel

PAGE 272

In this study, Jeong et al. report an 8.2 Å resolution cryo-electron microscopy 3D reconstruction of the AcrAB-TolC complex. The pseudoatomic structure demonstrates the assembly model based on the intermeshing cogwheel interaction between AcrA and TolC.

Caught in a Toxic Relationship

PAGE 277

Tse2 is a *Pseudomonas aeruginosa* Type 6 secretion system substrate and cytoactive toxin whose structural features suggest a relationship with ADP-ribosylating toxins and an active site arrangement consistent with NAD-dependent activity, providing the first insight into the molecular basis of Tse2 toxicity.

O_2-Tolerant H_2 Oxidation

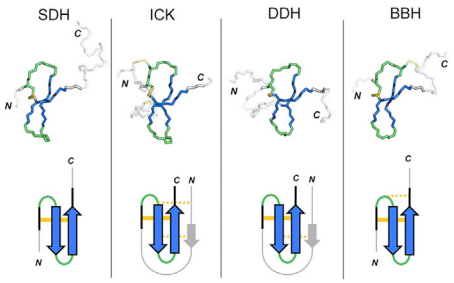
PAGE 285

Schäfer et al. report on the first crystal structure of a member of a peculiar group of O_2-tolerant, H_2-converting hydrogenases. Representatives of this novel group have shown to be able to oxidize even the traces of H_2 present in the atmosphere.

Single Disulfide-Directed β-Hairpin Fold—It's All New!

PAGE 293

Robinson et al. report the discovery of a new peptide fold they have called the single disulfide-directed β-hairpin (SDH). The SDH is a naturally occurring, small, highly stable, independent folding unit and is the common elementary motif underlying several peptide folds, including the inhibitor cystine knot.



Membrane Proteins Seeking Chaprones, Find Nanodiscs

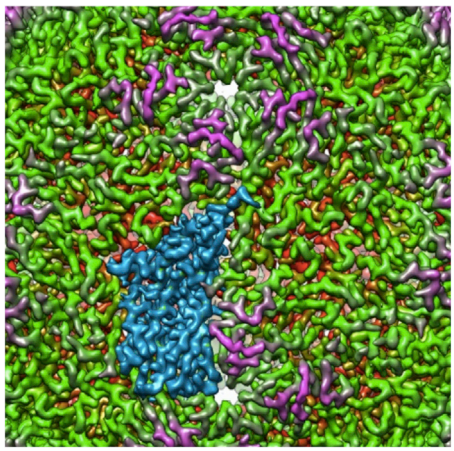
PAGE 300

Generation of affinity reagents for structural and functional characterization of membrane proteins is challenging in detergents. Dominik et al. describe an improved antibody phage display protocol for membrane proteins exploiting nanodiscs. This expands the usability of the method to multiple challenging membrane protein systems.

H/D Exchange Enters Gas Phase

PAGE 310

Mistarz et al. present the use of gas-phase H/D exchange mass spectrometry (gas-phase HDX-MS) to probe the binding-interface of protein-ligand complexes and measure the number of heteroatom-bound, non-amide, side-chain sites implicated in inter-molecular interactions in the complex. The novel approach is demonstrated for both protein-glycan and protein-peptide ligand complexes.



New Image Processing Strategy Gets Cryo-EM below 3 Å in 8 Hr

PAGE 319

Liu et al. develop an image processing strategy for single particle cryo-EM images of close-packed virus particles. This strategy was used to achieve a 2.9 Å resolution reconstruction of a 1.67 MDa virus-like particle of a circovirus, PCV2, recorded on 86 photographic films in 8 hr.

The Achilles' Heel of Aging Proteomes

PAGE 329

de Graff et al. show that random modification of side-chain charge by oxidative damage could be a dominant source of protein stability loss in aging organisms. This provides a mechanism connecting damage to functional loss and sheds light on the puzzle of how small levels of damage could affect aging.

Role of Lipid Interactions of the EphA2 Receptor

PAGE 337

Chavent et al. combine multiscale molecular dynamics simulations with a biochemical assay to describe the interactions of the EphA2 receptor FN2 domain with the anionic lipids of a model membrane. This provides insights into the dynamic behavior of the receptor at the cell surface.

